Renyi Thermostatistics and Self-Organization

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Abstract

Taking into account extremum of a Helmholtz free energy in the equilibrium state of a thermodynamic system the Renyi entropy is derived from the Boltzmann entropy by the same way as the Helmholtz free energy from the Hamiltonian. The application of maximum entropy principle to the Renyi entropy gives rise to the Renyi distribution. The q-dependent Renyi thermodynamic entropy is defined as the Renyi entropy for Renyi distribution. A temperature and free energy are got for a Renyi thermostatistics. Transfer from the Gibbs to Renyi thermostatistics is found to be a phase transition at zero value of an order parameter $\eta = 1-q$. It is shown that at least for a particular case of the power-law Hamiltonian $H = C\sum_i x_i^\kappa$ this entropy increases with η. Therefore in the new entropic phase at $\eta > 0$ the system tends to develop into the most ordered state at $\eta = \eta_{max} = \kappa/(1+\kappa)$. The Renyi distribution at η_{max} becomes a pure power-law distribution.

KEY WORDS: entropy bath, Renyi entropy, maximum entropy principle, order parameter, phase transition, self-organization.

1 Introduction

Numerous examples of power–law distributions (PLD) are well-known in different fields of science and human activity [1]. Power laws are considered [2] as one of signatures of complex self-organizing systems. They are sometimes called Zipf–Pareto law or fractal distributions. We can mention here the Zipf–Pareto law in linguistics [3], economy [4] and in the science of sciences [5], Gutenberg-Richter law in geophysics [6], PLD in critical phenomena [7], PLD of avalanche sizes in sandpile model for granulated media [8] and fragment masses in the impact fragmentation [9, 10], etc.

According to the well-known maximum entropy principle developed by Jaynes [11] for a Boltzmann-Gibbs statistics an equilibrium distribution of probabilities must provide maximum of the Boltzmann information entropy S_B upon additional conditions of normalization $\sum_i p_i = 1$ and a fixed average energy $U = \langle H \rangle_p \equiv \sum_i H_i p_i$.

Then, the Gibbs canonical distribution $\{p_i^{(G)}\}$ is determined from the extremum of the functional

$$L_G(p) = -\sum_i^W p_i \ln p_i - \alpha_0 \sum_i^W p_i - \beta_0 \sum_i^W H_i p_i, \tag{1}$$

where α_0 and $\beta_0 = 1/k_B T_0$ are Lagrange multipliers and T_0 is the thermodynamic temperature.

However, when investigating complex physical systems (for example, fractal and self-organizing structures, turbulence) and a variety of social and biological systems, it appears that the Gibbs distribution does not correspond to observable phenomena. In particular, it is not compatible with a power-law distribution that is typical [2] for such systems. Introducing of additional constraints on a sought distribution in the form of conditions of true average

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values $\langle X^{(m)}\rangle_p$ of some physical parameters of the system $X^{(m)}$ gives rise to a generalized Gibbs distribution with additional terms in the exponent but does not change its exponential form.

Montroll and Shlesinger [12] investigated this problem and found that maximum entropy principle applied to the Gibbs–Shannon entropy could give rise to the power–law distribution under only very special constraint that "has not been considered as a natural one for use in auxiliary conditions."

2 Helmholtz free energy and Renyi entropy

The well–known Boltzmann formula defines a statistical entropy, as a logarithm of a number of states W attainable for the system

$$S_W^{(B)} = \ln W \tag{2}$$

Here and below the entropy is written as dimensionless value without the Boltzmann constant k_B. Besides, we will use a natural logarithm instead of binary logarithm accepted in information theory.

This definition is valid not only for physical systems but for much more wide class of social, biological, communication and other systems described with the use of statistical approach. The only but decisive restriction on the validity of this equation is the condition that all W states of the system have equal probabilities (such systems are described in statistical physics by a microcanonical ensemble). It means that probabilities $p_i = p_W \equiv 1/W$ (for all $i = 1, 2, ..., W$) that permits to rewrite the Boltzmann formula as $S_W^{(B)} = -\ln p_W$. When the probabilities p_i are not all equal we can introduce an ensemble of microcanonical subsystems in such a manner that all W_i states of the i-th subsystem have equal probabilities p_i and its Boltzmann entropy is $S_i^{(B)} = -\ln p_i$. The simple averaging of the Boltzmann entropy $S_i^{(B)}$ leads to the Gibbs–Shannon entropy

$$S^{(G)} = \langle S_i^{(B)}\rangle_p \equiv -\sum_i p_i \ln p_i. \tag{3}$$

Just such derivation of $S^{(G)}$ is used in some textbooks (see, e. g. [13, 14])

This entropy is generally accepted in equilibrium and non-equilibrium statistical thermodynamics [15, 16] and communication theory but needs in modification for complex systems. To seek out a direction of modification of the Gibbs–Shannon entropy we consider first extremal properties of an equilibrium state in thermodynamics.

A direct calculation of an average energy of a system gives the internal energy U, its extremum is characteristic of an equilibrium state of rest for a mechanical system, other than a thermodynamic system that can change heat with a heat bath of a fixed temperature T_0. An equilibrium state of the latter system is characterized by extremum of the Helmholtz free energy F. To derive it statistically from the Hamiltonian $H = \sum_i H_i$ without use of thermodynamics we can following Balescu [17] introduce a moment-generating function

$$\Phi_H(\alpha) = \sum_i e^{\alpha H_i}, \tag{4}$$

where α is the arbitrary constant, and construct a cumulant-generating function

$$\Psi_H(\alpha) = \ln \Phi_H(\alpha) \tag{5}$$

that becomes the Helmholtz free energy F when divided by α that is chosen as $\alpha = -1/k_B T_0$.

Such a choice of the pre-factor $1/\alpha$ ensures a limiting passing of the Helmholtz free energy F into the internal energy U when $\alpha \to \infty$ ($T_0 \to 0$).

Now we return to the problem of a generalized entropy for open complex systems. Exchange by both energy and entropy (or information) with the environment is inherent in such systems (see e. g. the book [13] devoted to this subject).

It is pertinent to introduce the noun of an *entropy bath* (or *information bath*). Coupling with the entropy bath can be regarded as a necessary condition for self-organization of a complex system.

As a result of such coupling the system under consideration can not reach a state of thermodynamic equilibrium that is characterized by maximum of the Gibbs–Shannon entropy, derived by the simple averaging of the Boltzmann entropy. It is necessary to look for any other function to characterize its steady state resulted from the coupling with the entropy bath.

An effort may be made to find a "free entropy" of a sort by the same way that was used above for derivation of the Helmholtz free energy for a system coupled with a heat bath. The moment-generating function is introduced as

$$\Phi_S(\alpha) = \sum_i e^{\alpha S_i^{(B)}} \tag{6}$$

Then the cumulant-generating function is

$$\Psi_S(\alpha) = \ln \Phi_S(\alpha) = \ln \sum_i p_i^{-\alpha}. \tag{7}$$

To obtain the desired generalization of the entropy we are to find an α-dependent numerical pre-factor which ensures a limiting pass of the new entropy into the Gibbs–Shannon entropy. Such the coefficient is $1/(1+\alpha)$. Indeed, the new α-family of entropies

$$S(\alpha) = \frac{1}{1+\alpha} \ln \sum_i p_i^{-\alpha}. \tag{8}$$

includes the Gibbs–Shannon entropy as a particular case when $\alpha \to -1$.

Thus, it has appeared that the desired "free entropy" coincides with the known Renyi entropy [18]. It is conventional to write it with the parameter $q = -\alpha$ in the form

$$S_q^{(R)}(p) = \frac{1}{1-q} \ln \sum_i p_i^q \tag{9}$$

On the other hand, we can represent Eq. (6) as

$$\Phi_S(q) = \sum_i p_i e^{(1-q) S_i^{(B)}} \tag{10}$$

Then the Renyi entropy can be represented as a particular case of the Kolmogorov–Nagumo [19, 20] generalized averages

$$\langle x \rangle_\phi = \phi^{-1} \left(\sum_i p_i \phi(x_i) \right) \tag{11}$$

if we put there the Kolmogorov–Nagumo function in the form $\phi(x) = \exp\{(1-q)x\}$, $\phi^{-1}(x) = \ln x^{1/(1-q)}$ and choose $x_i = \ln S_i^{(B)}$.

Renyi introduced his entropy just in such a manner. Renyi wanted to find the most general class of entropies which preserved the additivity for statistically independent systems and was compatible with the Kolmogorov–Nagumo generalized average. By this way he found the exponential Kolmogorov–Nagumo function $\phi(x)$. Physically, such a choice of $\phi(x)$ on its own appears accidental until it is not pointed to the fact that the same exponential function of the Hamiltonian provides derivation of the free energy which is extremal in an equilibrium state of a thermodynamic system exchanging heat with a heat bath. This fact permits us to suppose that the Renyi entropy derived in the same manner should be extremal at a steady state of a complex system which exchange entropy with its surroundings actively.

Note that for linear $\phi(x) = cx + d$ the Kolmogorov–Nagumo generalized average turns out to be the ordinary linear mean and hence the Gibbs-Shannon entropy follows as an average entropy in the usual sense.

3 Axiomatical foundation of the Renyi entropy

In view of the way of the Renyi entropy derivation we can suppose that it is maximal at a steady state of a complex system being in contact with the entropy bath. Such a supposing is justified by the Shore–Johnson theorem [21, 22, 23]. They considered a procedure of updating of a distribution function when a new information related to the system had appeared in a form of an additional constraint I .

Shore and Johnson gave five "consistency axioms" for this updating operation [21, 22]: 1) Uniqueness: The result should be unique. 2) Invariance: The choice of coordinate system should not matter (for continuous probability densities).3) System independence: It should not matter whether one accounts for independent information about independent systems separately in terms of different densities or in terms of a joint density. 4) Subset independence: It should not matter whether one treats disjoint subsets of system states in terms of separate conditional densities or in terms of the full density. 5) In the absence of new information, we should not change the prior.

The following theorem is proven on the base of these axioms (here it is for the particular case of a homogeneous prior distribution $u_i = 1/W$ (for all i)):

Theorem *An updating procedure satisfies the five consistency axioms above if and only if it is equivalent to the rule*

Maximize

$$U_\eta(p) = (\sum_i^W p_i^{1-\eta})^{1/\eta}, \ (\eta < 1)$$

under the constraint I *.*

or

Maximize any monotonous function $\Psi(U_\eta(p))$ *under the constraint* I *.*

The most evident choice of the monotonous function is $\Psi(U_\eta) = \ln U_\eta(p)$, that is the Renyi entropy $S_q^{(R)}$ for $q = 1 - \eta$. Such a choice of Ψ ensures the limit $S_q^{(R)} \to S^{(G)}$ when $q \to 1$ and passage of $S_q^{(R)}$ (for all q) to $S_W^{(B)}$ in the case of absence of new information when $p_i = u_i = 1/W$ (for all i). Both these properties should be considered as necessary conditions for a choice of $\Psi(U_\eta)$. In particular, the function $\Psi_T(U_\eta) = (U_\eta^\eta - 1)/\eta$ leading to the Tsallis entropy fails because it does not satisfy the second of these conditions.

Thus, the Shore-Johnson theorem provide quite conclusive foundation of the Renyi entropy as itself and the maximum entropy principle for it and in doing so it justifies the

above proposal that the Renyi entropy as the free entropy is maximal at a steady state of a complex system.

In the light of this theorem the Khinchin's uniqueness theorem [24] for the Gibbs–Shannon entropy should be reconsidered. Khinchin based on the next three axioms:
(1) $S(p)$ is a function of the probabilities p_i only and has to take its maximum value for the uniform distribution of probabilities $p_i = 1/W$: $S(1/W, ..., 1/W) \geq S(p')$, where p' is any other distribution.
(2) The second axiom refers to a composition Σ of a master subsystem Σ^I and subordinate subsystem Σ^{II} for which probability of a composed state is

$$p_{ij} = Q(j|i)p_i^I \tag{12}$$

where $Q(j|i)$ is the conditional probability to find the subsystem Σ^{II} in the state j if the master subsystem Σ^I is in the state i . Then the axiom requires that

$$S(p) = S(p^I) + S(p^I|p^{II}) \tag{13}$$

where

$$S(p^I|p^{II}) = \sum_i p_i^I S(Q|i) \tag{14}$$

is the conditional entropy and $S(Q|i)$ is the partial conditional entropy of the subsystem Σ^{II} when the subsystem Σ^I is in the i -th state.
(3) $S(p)$ remains unchanged if the sample set is enlarged by a new, impossible event with zero probability: $S(p_1, ..., p_W) = S(p_1, ..., p_W, 0)$

While proving his uniqueness theorem Khinchin enlarged the second axiom. He supposed that all U states of the composite system Σ were equally probable, that is, $p_{ij} = 1/U$ for all i and j ; whence he got

$$S(p) = \ln U \tag{15}$$

Besides, Khinchin supposed that U_i^{II} states of the subsystem Σ^{II} corresponding to each i -th state of the master subsystem Σ^I are equally probable, as well. So, he took $Q(j|i) = 1/U_i^{II}$ for $i = 1, ..., W$ and $j \in U_i^{II}$; whence from Eqs. (12) and (14) he obtained $U_i^{II} = Up_i^I$ and

$$S(Q|i) = \ln U_i^{II}, \quad S(p^I|p^{II}) = \ln U + \sum_i p_i^I \ln p_i^I. \tag{16}$$

Substituting Eqs. (15), (16) into Eq. (13) Khinchin got the Gibbs–Shannon entropy for the master subsystem Σ^I $S^{(G)}(p^I) = -\sum_i^W p_i^I \ln p_i^I$. It should be noted that the last Khinchin's supposition of equal probabilities of states of the subsystem Σ^{II} is the most questionable and should be abandoned. Indeed, the probability distribution for Σ^{II} coupled with the master subsystem should be rather canonical distribution than equally probable one. On the other hand, the abandonment of this supposition destroys all the proof of the Khinchin theorem.

So, we are left with only the Shore–Johnson theorem where the Gibbs–Shannon entropy is no more than a particular case of the Renyi entropy.

4 The Renyi thermostatistics

The maximum entropy principle for the Renyi entropy $S^{(R)}$ under additional constraints of fixed value $U = \langle H \rangle_p \equiv \sum_i H_i p_i$, and normalization of p gives rise [25, 26] to the Renyi

distribution function

$$
\begin{aligned}
p_i &= p_i^{(R)} = Z_R^{-1}\left(1-\beta\frac{q-1}{q}\Delta H_i\right)^{\frac{1}{q-1}} \qquad (17)\\
Z_R &= \sum_i\left(1-\beta\frac{q-1}{q}\Delta H_i\right)^{\frac{1}{q-1}}, \ \Delta H_i = H_i - U.
\end{aligned}
$$

At $q \to 1$ the distribution $\{p_i^{(R)}\}$ becomes the Gibbs canonical distribution in which the constant $\beta = 1/k_B T_0$.

Substituting the Renyi distribution (17) into the Renyi entropy definition (9), we find the thermodynamic entropy in the Renyi thermostatistics as

$$
\tilde{S}_q^{(R)} = S_q^{(R)}(p_q^{(R)}) = k_B \ln Z_q^{(R)}. \qquad (18)
$$

where the Boltzmann constant k_B is introduced.

When $q \to 1$ this entropy passes into thermodynamic entropy in the Gibbs thermostatistics

$$
\tilde{S}^{(G)} = S^{(G)}(p^{(G)}) = k_B \ln \sum_i^W e^{-\beta \Delta H_i}. \qquad (19)
$$

On the other hand, the Gibbs thermostatistics is based on the Gibbs distribution for energy H_i but not fluctuations of energy ΔH_i . So, the Renyi distribution (17) should be represented as a distribution for energy H_i , as well. Dividing both the expression in the brackets in Eq. (17) and Z_R by $(1-(1-q)\beta U/q)^{1/(q-1)}$ we get the alternative equivalent form of the Renyi distribution

$$
p_i^* = Z_*^{-1}\left(1+\frac{1-q}{q}\beta^* H_i\right)^{\frac{1}{q-1}} \qquad (20)
$$

$$
Z_* = \sum_i\left(1+\frac{1-q}{q}\beta^* H_i\right)^{\frac{1}{q-1}}, \ \beta^* = \frac{\beta}{1-\frac{1-q}{q}\beta U}
$$

The thermodynamic Renyi entropy can be represented in the alternative form, as well

$$
\begin{aligned}
\tilde{S}_q^{(R)}(p^*) &= \frac{k_B}{1-q}\ln\sum_i p_i^{*q}\\
&= \frac{k_B}{1-q}\ln\left(1+\frac{1-q}{q}\beta^* U\right) + k_B \ln Z_* \qquad (21)
\end{aligned}
$$

A physical q-dependent temperature in the Renyi superstatistics should be defined in a standard manner as

$$
T_q = \left(\frac{\partial S_q^{(R)}}{\partial U}\right)^{-1} = \left(\frac{k_B}{q}\frac{\beta^*}{1+\frac{1-q}{q}\beta^* U}\right)^{-1} = \frac{q}{k_B \beta}. \qquad (22)
$$

It was shown [25] that $\beta = \beta_0$ at least for the power-law Hamiltonian, so the physical q-dependent temperature becomes $T_q = qT_0$ where T_0 is the temperature of a heat bath. According to Ref. [27], the fact that $T_q < T$ $(q < 1)$ says in favor of greater ordering of states with lower q .

The Helmholtz free energy is defined in the Renyi thermostatistics as

$$
F^{(R)} = -k_B T_q \ln Z_*. \qquad (23)
$$

On the other hand, the thermodynamic definition of the free energy should be

$$\tilde{F} = U - T_q \tilde{S}^{(R)}. \tag{24}$$

It is not difficult to ensure that both definitions coinside in the limit $q \to 1$. For arbitrary q , their equivalence can be checked for the particular case of the power-law Hamiltonian. With the use of the relation $\beta U = 1/\kappa$ [25] we get $\tilde{F} - F^{(R)} = C_q T_q$ where

$$C_q = 1/(q\kappa) - \ln[1 - (1-q)/(q\kappa + q - 1)]/(1-q). \tag{25}$$

Such a difference can not provoke objections because of the free energy is determined in thermodynamics with an accuracy of an addent $C_1 T + C_2$.

5 Entropic phase transition

Thus, we have Gibbs and Renyi thermostatistics based on different microscopic entropy definitions. Each of them provides an adequate description of corresponding class of systems and we need in a rigorous formulation of conditions of transfer from one thermostatistics to another.

Transfer from the Gibbs distribution describing a state of dynamic chaos [27] to power–law Renyi distributions that are characteristic for ordered self-organized systems [2] corresponds to an increase of an "order parameter" $\eta = 1 - q$ from zero at $q = 1$ up to $\eta_{max} = 1 - q_{min}$.

In accordance to the Landau theory [28] of phase transitions an entropy derivative with respect to the order parameter undergoes a jump at a point of the phase transition.

Here we deal with the transfer from the Gibbs thermostatistics to the Renyi thermostatistics corresponding to non-zeroth values of the order parameter η . Let us consider a variation of the entropy at this transition.

Now it is not difficult to calculate the limiting value at $\eta \to 0$ of the derivative of the entropy $\tilde{S}_\eta^{(R)}$ with respect to η . We get

$$\lim_{\eta \to 0} \left(\frac{d\tilde{S}^{(R)}}{d\eta} \right) = \frac{k_B}{2} \beta^2 \sum_i^W p_i^{(G)} \left(\Delta H_i \right)^2 \tag{26}$$

According to a fluctuation theory for the Gibbs equilibrium ensemble we have

$$\sum_i^W p_i^{(G)} \left(\Delta H_i \right)^2 = \frac{1}{k_B \beta^2} \frac{dU}{dT} = \frac{1}{k_B \beta^2} C_V \tag{27}$$

whence

$$\lim_{\eta \to 0} \left(\frac{d\Delta \tilde{S}}{d\eta} \right) = \frac{1}{2} C_V. \tag{28}$$

where C_V is the heat capacity at a constant volume.

Thus, the derivative of the entropy gain with respect to the order parameter exhibits the jump (equal to $C_V/2$) at $\eta = 0$. This permits us to consider the transfer to the Renyi thermostatistics as a peculiar kind of a phase transition into a more organized state. We can give this transition the name *entropic phase transition.*

As a result of the entropic phase transition the system passes into an ordered state with the order parameter $\eta \neq 0$. In contrast to the usual phase transition that takes place at the temperature of phase transition, conditions of the entropic phase transition are likely to

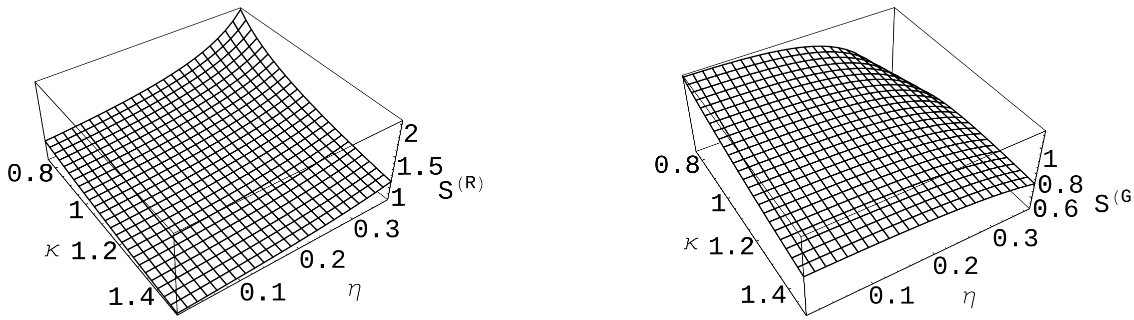

Figure 1: The landscapes of the entropies $\tilde{S}_{\eta}^{(R)}[p^{(R)}(\eta,\kappa)]$ (left) and $\tilde{S}^{(G)}[p^{(R)}(\eta,\kappa)]$ (right) for the power–law Hamiltonian with the exponent κ and $\eta < \kappa/(1+\kappa)$.

be determined partially for each concrete system. For example, a threshold of emergence of turbulence (see [29]) as an ordered structure is determined by a critical Reynolds number and an emergence of Benard cells is determined by a critical Rayleigh number (see [27]).

Social, economical and biological systems are realized as a rule in ordered self–organized forms. This is the reason why power–law and closely related distributions are characteristic for them but not canonical Gibbs distribution.

For the particular case of a power–law Hamiltonian $H_i = Cx_i^{\kappa}$ problem of a value of the order parameter was discussed in Ref. [25] where maximum maximorum of the thermodynamic Renyi entropy was found at $q = q_{min} = 1/(1+\kappa)$, that is, at $\eta = \eta_{max} = \kappa/(1+\kappa)$. The Renyi distribution for such η_{max} becomes a pure power–law distribution that agrees with observable data for self-organized systems.

The landscapes of this entropy $\tilde{S}_{\eta}^{(R)}[p^{(R)}(\eta,\kappa)]$ is illustrated in Fig. 1 (left). The landscape of the usual thermodynamic Gibbs entropy $S^{(G)}[p^R(x|q,\kappa)]$ for the same Renyi distribution is illustrated in Fig. 1 (right). It is seen that in contrast to $\tilde{S}_{\eta}^{(R)}[p^{(R)}(\eta,\kappa)]$ the Gibbs entropy $S^{(G)}[p^R(x|q,\kappa)]$ decreases with the gain of η and attains its maximum at $\eta = 0$, that is in the most disordered state when the Renyi distribution becomes the Gibbs canonical one.

6 Conclusion

It should be stressed that thermodynamic laws are irrelevant to microscopic interpretations of thermodynamic functions. On the other hand, according to the Boltzmann–Gibbs microscopic interpretation of entropy, its gain is accompanied by evolution of a system to an homogeneous equilibrium state of thermal chaos. In contrast, the Renyi thermodynamic entropy increases as a system ordering (departure of the order parameter η from zero) increases (see Fig. 1). So, it can be considered as a kind of potential that drives the system to self-organized state.

Transfer from the usual Gibbs thermostatistics to the Renyi thermostatistics takes the form of a phase transition of ordering with the order parameter η . As soon as the system passes into this new phase state of the Renyi thermostatistics, a spontaneous development of self–organization to a more ordered state begins accompanied with gain of thermodynamic entropy. In doing so the well-known contradiction between observable spontaneous self–organization and the Second Law is eliminated when we use the Renyi entropy as a

microscopic definition of the thermodynamic entropy instead of the Gibbs–Shannon one.

Moreover, it may be supposed that biological evolution or development are governed by the extremal principle of the Renyi thermostatistics.

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